Energy Conversion and Combustion Sciences

Date: 08 March 2013

Chiping Li
Program Officer
AFOSR/RTE
Air Force Research Laboratory

Integrity ★ Service ★ Excellence

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NAME: **CHIPING LI**

<u>BRIEF DESCRIPTION OF PORTFOLIO</u>:

Meet *Basic Combustion Challenges* with *New Approaches*
Explore *New Energy Conversion Opportunities* for
Next Generation Air Force Propulsion Systems of Game-Changing Efficiency and Operability

Key Portfolio Attributes*:*

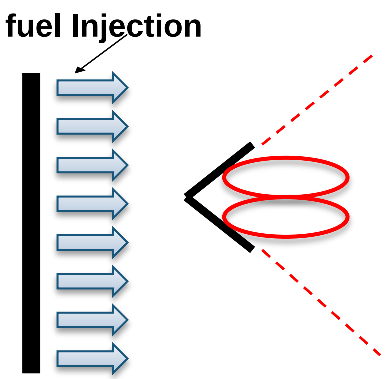
- •Understand *Fundamentals* in Realms of *Air Force* Interests (understand the nature as it is)
- •Quantify *Rate-Controlling* Processes and Scales in Multi-Physics, Multi-Scale Phenomena (find ways to control complex phenomena)

<u>LIST SUB-AREAS IN PORTFOLIO</u>:

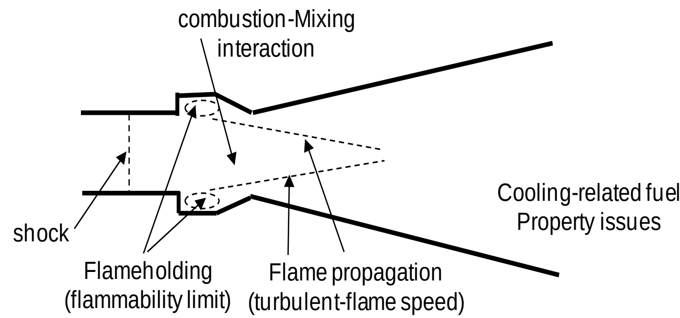
1. Combustion Chemistry (underlying chemistry, new approaches -- working with Drs. Berman/RTE, ARO & DOE/BES)
2. Turbulent Flame Properties/Models (nonlinear flow-chemistry interaction, new thinking/tools)
3. Combustion Numerics (new tools -- collaborating with Dr. Fariba/RTA)
4. Combustion Diagnostics (new tools -- collaborating with Dr. Parra/RTB)
5. Game-Changing Energy Conversion Concepts (new opportunities, Drs. Berman/RTE, Luginsland/RTB, & ONR)

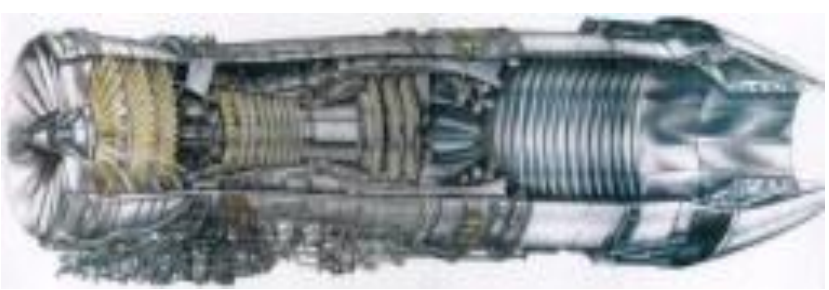
Sub-areas are multi-disciplinary: collaboration with other POs & Agencies are essential.

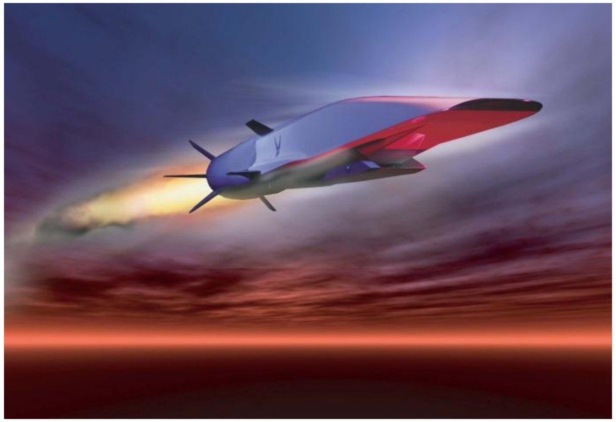
- ***Most Important*** determining factors of operability and performance;
- ***Least Understood*** areas in basic combustion research, with large uncertainties;
- Confluence of “grand-old” fundamental science challenges, immediate needs and long-term interests.



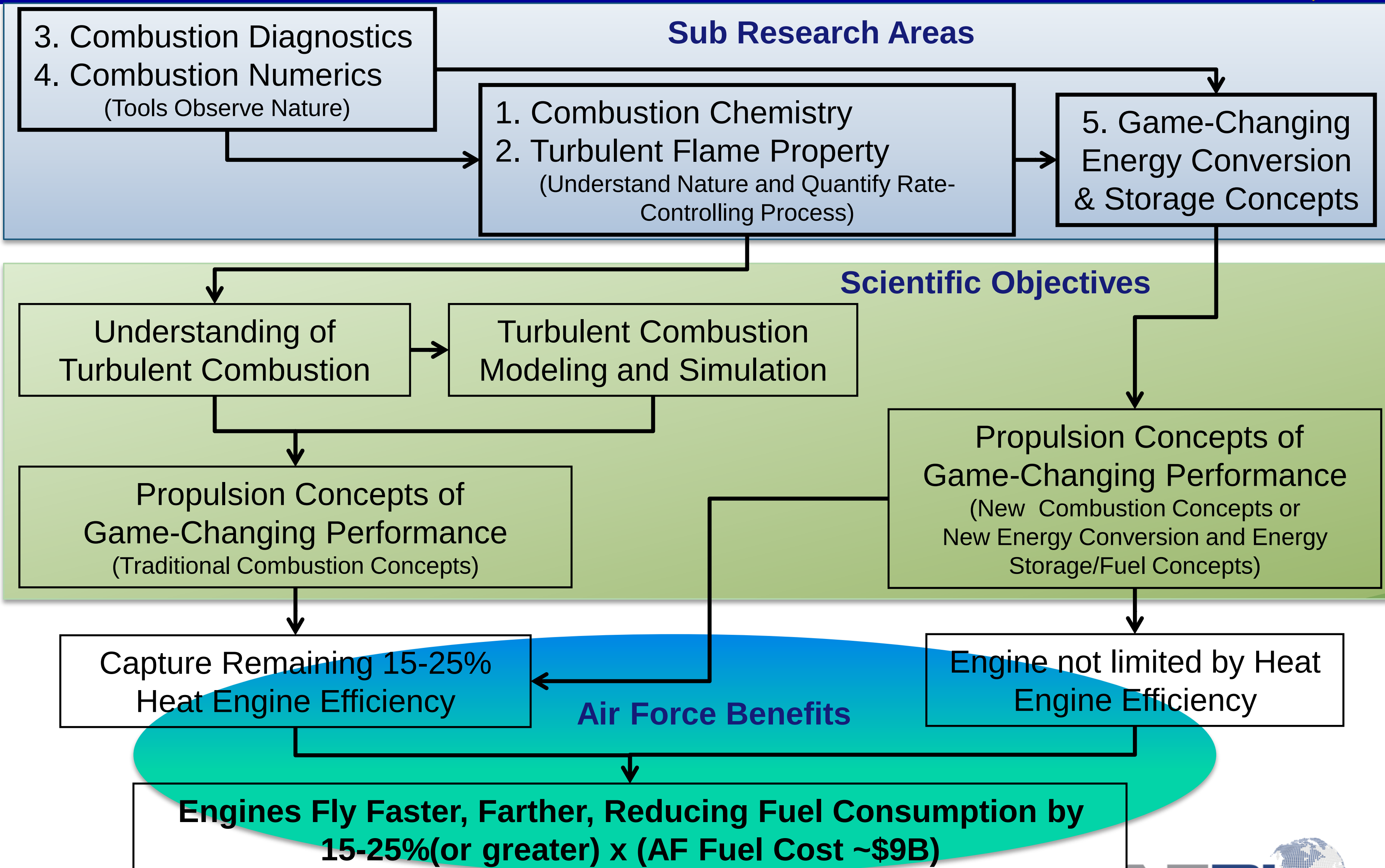
Cavity Based Scramjet Combustor







Portfolio Logic and Strategy



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Portfolio Directions/Trends

1. **Combustion Chemistry**
   - Reaction-pathway centric approaches (based on ab initial methods and exp. data)↑
   - Traditional detailed reaction-rate-constant centric approaches ↓

2. **Turbulent Flame Properties/Models**
   - Turbulent flame experiments in realm of AF interests (high-Re, compressible) ↑
   - Laminar and weakly turbulent flame experiments↓
   - Scale interaction models based on DNS, experimental data and new math approach↑
   - Models based on assumptions not directly verifiable by experiments ↓

3. **Combustion related Numerical Techniques**
   - Coupled simulation-experiment approaches↑
   - Computational methods for studying stochastic pathways↑
   - Computational methods for reduction of “large” detailed combustion chemistry models↓

4. **Combustion Diagnostics**→

5. **Game-Changing Energy Conversion Concepts**
   - New combustion concepts→
   - Direct/partially direct conversion from chemical energy to mechanical energy↗
   - New energy-storage/ fuel concepts for propulsion application ↗

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Coordination with Other Agencies

1. **Strong collaboration is continuously being forged in following areas:**
   - Diagnostics (Mainly DoE, NASA)
   - Numerical (DoE, NASA, ARO)
   - Combustion Chemistry (DoE, ARO, NSF)
   - Innovative Combustion Concept (ONR, ARO)

2. **Dividing problems and condition areas according to each interests:**
   - AFOSR combustion portfolio:
     - Turbulence combustion area: Air-Force relevant realms, i.e. compressible, high-Re conditions for propulsion applications
     - Combustion Chemistry: Reaction-pathway centric approaches
   - DOE -- a well funded combustion program focusing on basic energy research:
     - turbulence combustion area: ground-base energy systems and auto-engine types of applications at relatively low-speed and low-Re conditions (TNF etc.)
     - combustion chemistry: large, detailed reaction-rate-constant centric approach
   - NASA -- a modest combustion program focusing:
     - "Very-high" speed (space access) region
     - Overlapping interests and close coordination with AF programs (scramjet, rockets etc.).
   - NSF -- a modest combustion program:
     - Covers broad ranges of combustion problems

3. **Multi-Agency Coordinate Committee of Combustion Research (MACCCR)**
   - Functioning well and its positive roles will continue

Multi-Agency Collaboration Benefits Every One

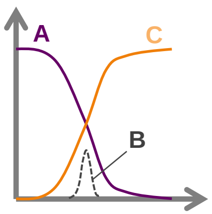
Combustion Chemistry

a New Direction

Combustion Chemistry: History and Recent Progress

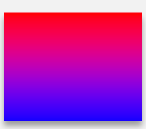
Spalding used 3-step "fictitious" reactions to describe the global reaction kinetics of a flame (*Philos. Trans. Royal Soc. London A* 1956)

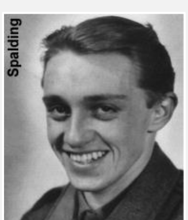
$$A \longrightarrow 2B \quad -66\ \text{kcal/mole} = \text{radical-producing},$$
$$B + A \longrightarrow B + 2C + 33\ \text{kcal/mole} = \text{chain},$$
$$B + B + X \longrightarrow 2C + X + 99\ \text{kcal/mole} = \text{chain-breaking}.$$



add physics

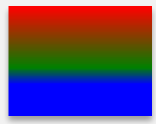
1950s'
Three-step, global chemistry with detailed transport



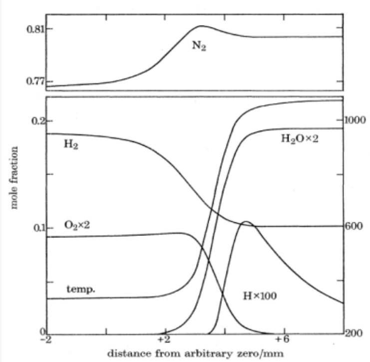


D. Brian Spalding

Late 60s-early 70s
remove empiricism by using ~10-20 step elementary chemistry

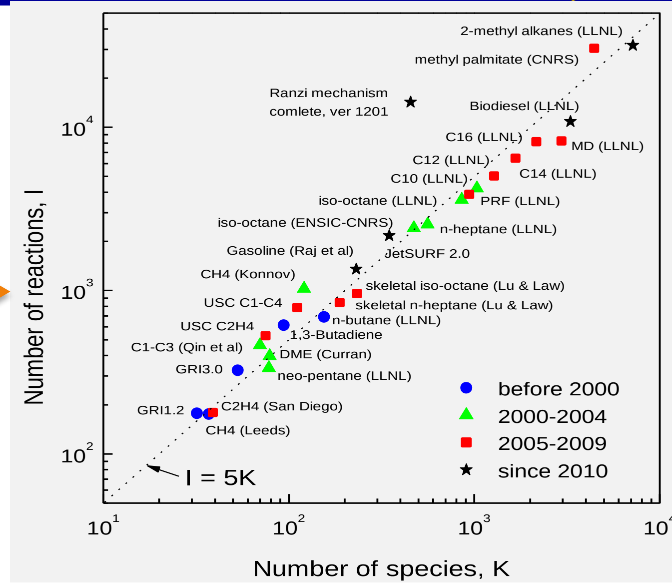


Graham Dixon-Lewis



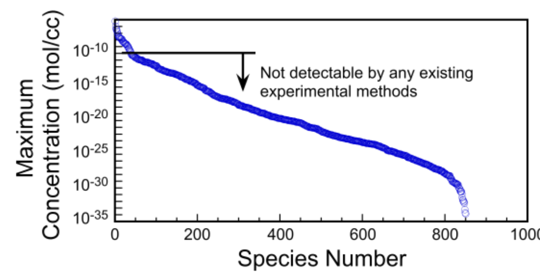
Dixon-Lewis' calculation of the structure of a hydrogen flame, including intermediate radical concentrations, using detailed chemistry (*Proc. R. Soc. Lond. A* 1970)

add physics or just follow the formula?



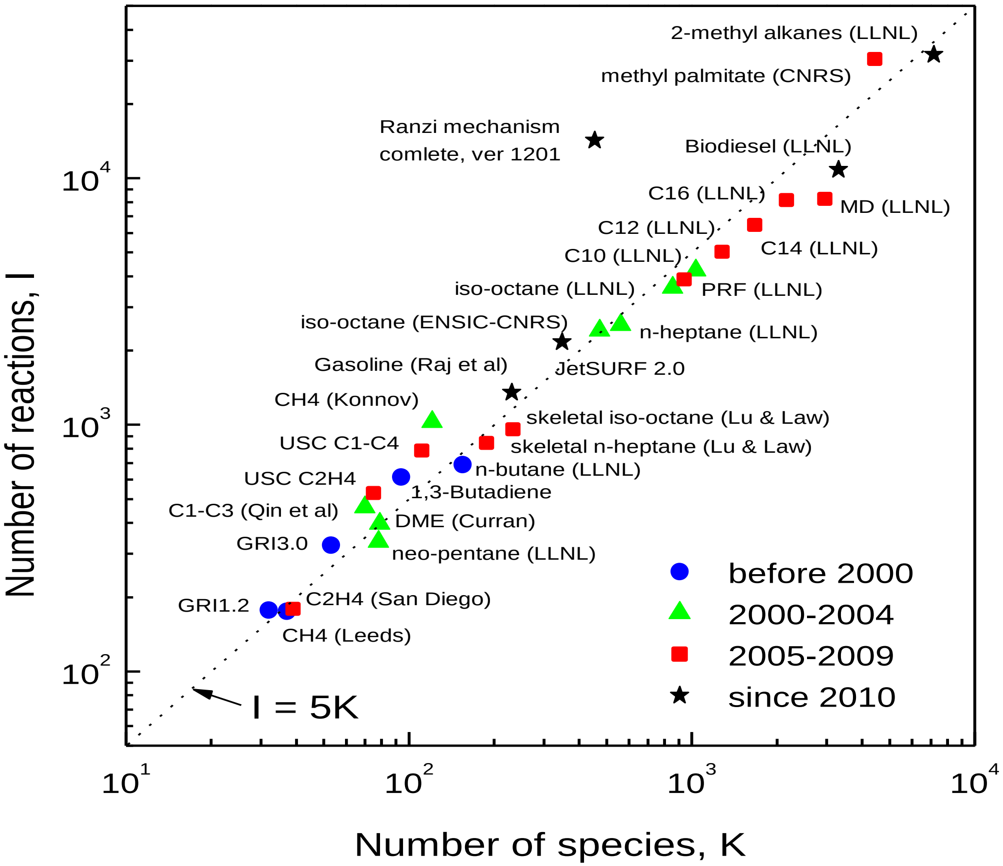
Today: following the formula, an extrapolation of Dixon-Lewis' work, but this is sure not what Dixon-Lewis had in mind.

- O(10^4) species and O(10^5) reactions with rates and pathways unverifiable.
- Back to the empirical past: > 90% species considered are not detectable by any experimental means.



Ranked maximum concentrations of species computed as an initial value problem using a typical reaction mechanism (T_0 = 1400 K and P = 1 atm)

Uncertainty vs. Model Size



The larger, the better – Maybe Not

Does the model uncertainty reduce as the model size grows – Not Necessarily

- **Uncertainties of Model inputs**
- **Uncertainties with model complexity**
- **Relationship between model size and its uncertainty**

Find out optimal model size for minimal uncertainty --- new direction in UQ for the combustion chemistry model

Two Distinctive, Complementary Approaches for Real HC Fuel

Traditional/State of Art "Rate Constants Centric"

(1) INCLUDE: combinatory approaches (up to **~ 10^4-10^5** reaction steps for common HC fuels)

(2) ESTIMATE: rate constants for most and calculate and measure for some

(3) SELECT: through sensitivity analysis, targeting ~ order of **10^2** reaction steps

Note1: large uncertainty in steps 1 & 2

Note2: There is a confusion between approximate natures of those large, complex reaction sets and exact nature of the human Genome set.

In the combustion process, reactions follow uncertain **pathways**, step by step.

$$k(T) = AT^n e^{-Ea/RT}$$

At each step in traditional Arrhenius model, the reaction rate is controlled by **rate constants.**

No.	reaction[b]		$k = A\,T^n \exp(-E/RT)$[c] A	n	E	references/ comments
	Reactions of propene					
1	$aC_3H_5 + H\ (+M) = C_3H_6\ (+M)$		2.00×10^{14}			k_∞, *d*
			1.33×10^{60}	–12.0	5968	k_0
		a=0.020	T^{***}=1097	T^{*}=1097	T^{**}=6860	*e*
2	$CH_3 + C_2H_3\ (+M) = C_3H_6\ (+M)$		2.50×10^{13}			k_∞, *f*
			4.27×10^{58}	–11.94	9770	k_0
		a= 0.175	T^{***}=1341	T^{*}=60000	T^{**}=10140	*e*
3	$C_3H_6 + H = C_2H_4 + CH_3$		1.60×10^{22}	–2.39	11180	1 atm, *g*
4	$C_3H_6 + H = aC_3H_5 + H_2$		1.70×10^{05}	2.5	2490	[33]
5	$C_3H_6 + H = CH_3CCH_2 + H_2$		4.00×10^{05}	2.5	9790	[33]
6	$C_3H_6 + O = CH_2CO + CH_3 + H$		1.20×10^{08}	1.65	327	[33]
7	$C_3H_6 + O = C_2H_5 + HCO$		3.50×10^{07}	1.65	–972	[33]
8	$C_3H_6 + O = aC_3H_5 + OH$		1.80×10^{11}	0.7	5880	[33]
9	$C_3H_6 + O = CH_3CCH_2 + OH$		6.00×10^{10}	0.7	7630	[33]
10	$C_3H_6 + OH = aC_3H_5 + H_2O$		3.10×10^{06}	2.0	–298	[33]
11	$C_3H_6 + OH = CH_3CCH_2 + H_2O$		1.10×10^{06}	2.0	1450	[33]
12	$C_3H_6 + HO_2 = aC_3H_5 + H_2O_2$		9.60×10^{03}	2.6	13910	[33]
13	$C_3H_6 + CH_3 = aC_3H_5 + CH_4$		2.20×10^{00}	3.5	5675	[33]
14	$C_3H_6 + CH_3 = CH_3CCH_2 + CH_4$		8.40×10^{-01}	3.5	11660	[33]

New/Start Exploring "Follow the Pathway"

(1) SELECT: identify important pathways following PES

(2) INCLUDE: only include most relevant ones – targeting no more than ~order of **10^2** reaction steps

(3) **OBTAIN:** rate constants from experimental measure and ab initio calculations

Note1: understanding of initial fuel break-up is most important

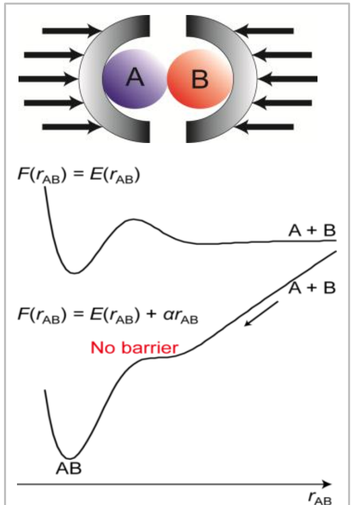
Note2: made possible for recent develop in diagnostics and ab. initio chemistry calculation method

? – Just Start Exploring

Combustion Chemistry Models of limited reaction steps with acceptable uncertainties, usable for reactive CFD tools

???? – Have Explored for more than forty years

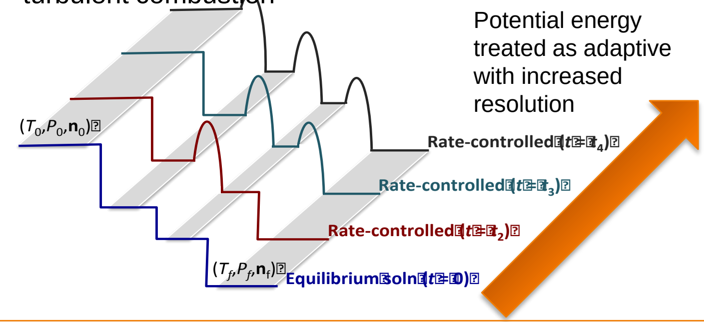
Ab. Initio Methods to Identify Key Pathways



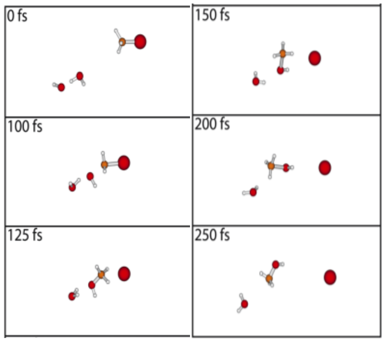
Artificial force induced reaction (AFIR) method

automated PES/PEL generation

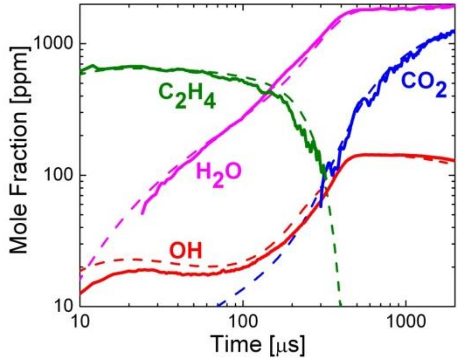
PEL-RCCE algorithm to enable application of PES in turbulent combustion



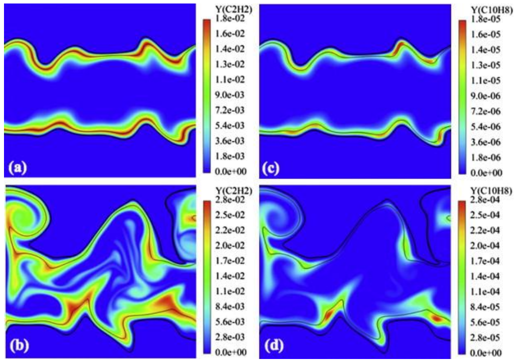
Chemical Dynamics



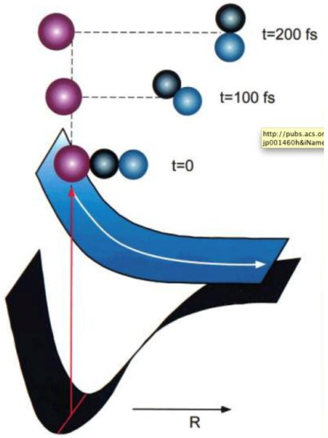
Experimental Validation



Combustion



Diagnostics in Combustion Chemistry



Femtochemistry

A + BC → [ABC]* → AB + C

Zewail, JPC A 104, 5660 (2000)

Heart beat

Picture refresh in LED TV

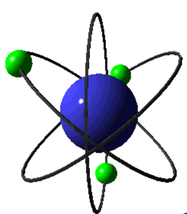
Period of AM radio

Computer processor speed

Molecular rotation

Molecular vibration

Electronic motion



1 second

10^{-3} milisec

10^{-6} microsec

10^{-9} nanosec

10^{-12} picosec

10^{-15} femtosec

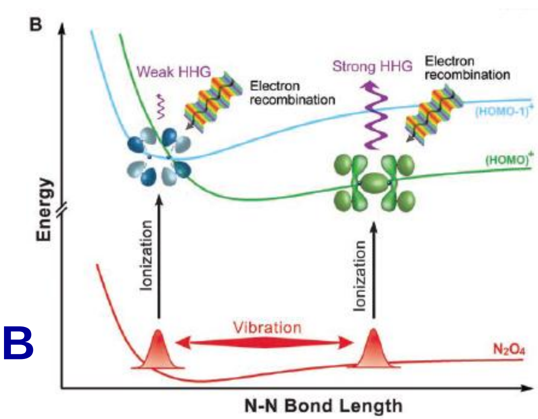
10^{-18} attosec

10^{-21} zeptosec

Attosecond physics/chemistry

A + B → [AB]* + e⁻ → AB

Murnane, Science 322, 1207 (2008)



Gord et. al., AFRL

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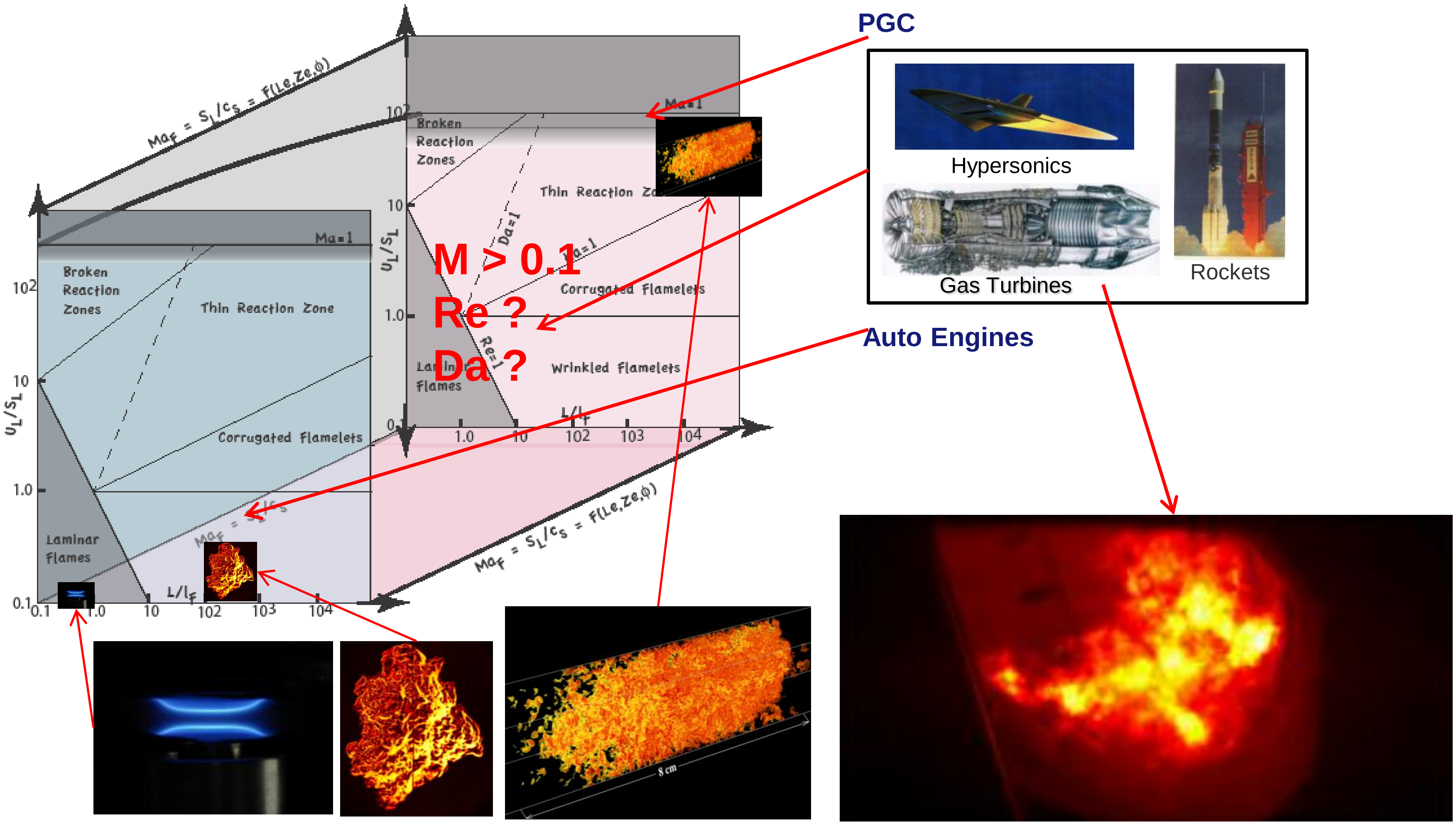
Combustion Chemistry: Where We Are

With recent developments in combustion diagnostics (especial ultra-fast lased based diagnostics) and ab. initio chemistry methods, we have unprecedented opportunities in combustion chemistry, --- AFOSR is leading the charge

leading to usable models with acceptable uncertainty to revolutionized Air Force propulsion system development.

Turbulent Flame Property
in Air-Force-Relevant Realms

Turbulence Combustion: Fundamental Structures, Critical Scales and Relevant Conditions



laminar flame | wrinkled flame ball | Hi-M, Hi-Re (flame brushes)

(1)Little Understanding and Data Available at AF Relevant Compressible, High-Re Conditions;
(2)Needs for Better Definition of Re-Conditions in Regions of Interests

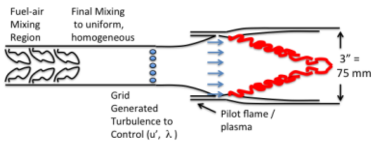
High-Re, Compressible Turbulence Flame Experiments at AF Relevant Condition Ranges

•Focus on key combustion properties and characteristics such as:

- ***•Flame propagation,***
- ***•Flammability limit***
- ***•Combustion instability***

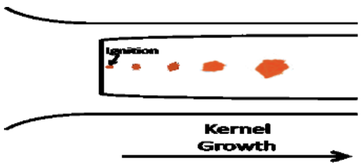
•Multi-phase conditions ***applicable*** to Air Force propulsion systems

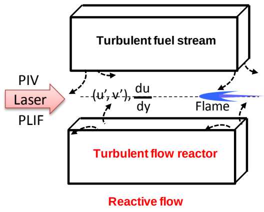
•Made possible by diagnostics developed by this portfolio up to date



Key Requirements (Experimental Data Objectives):

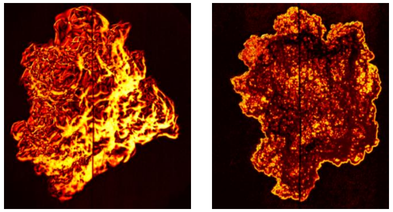
1. ***Understanding*** the above key combustion phenomena and characteristics;
2. ***Quantifying rate-controlling processes and scale****s* that govern those phenomena and characteristics;
3. Developing and validating as directly as possible ***basic model assumptions***
4. Controlling and quantifying turbulence properties are ***essential***.





Proposals are being considered and funded for:

- •Defining relevant conditions and Studying Critical Scales (1 funded in FY12)
- •Relevant Experiments in different configurations (4 funded in FY12)

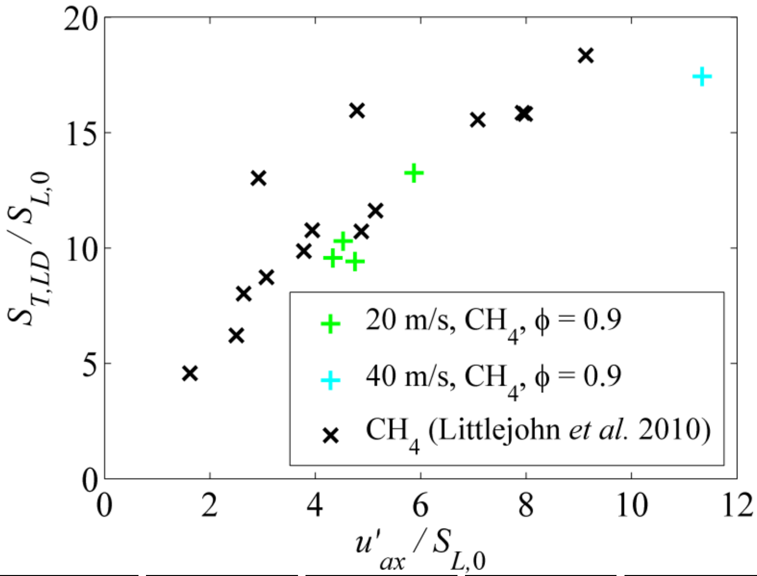


Understanding Nature from Observation and Data

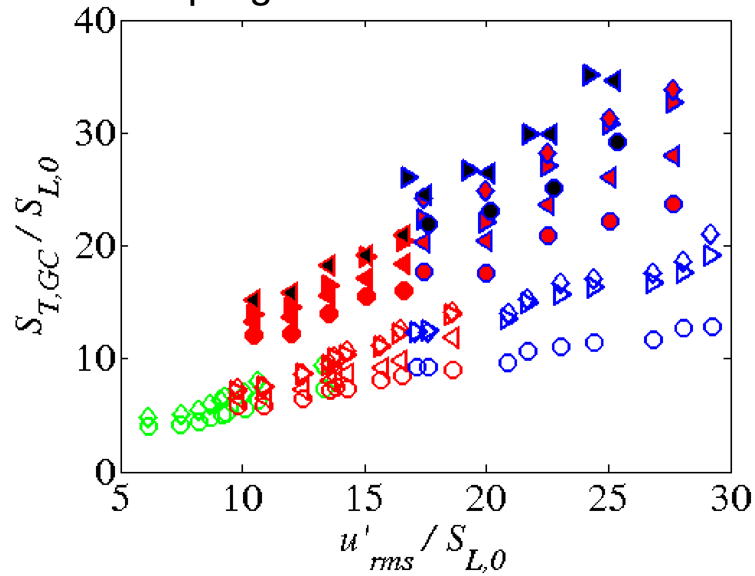
More Turbulent Flame Experiments

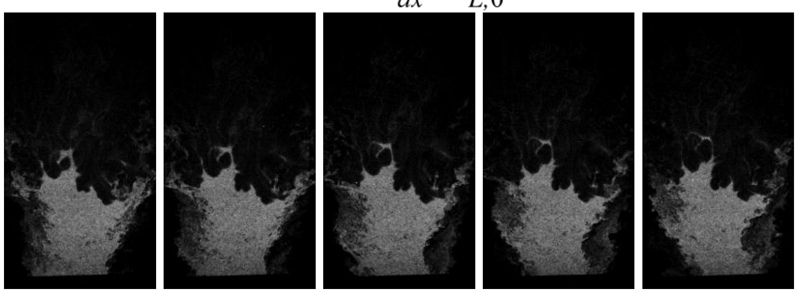
Speed and Free Propagating Turbulent Flame and Swirl Flame: (PI: Lieuwen, Georgia Tech)

swirl burner (jet-engine similar) data



sister program Bunsen burner data





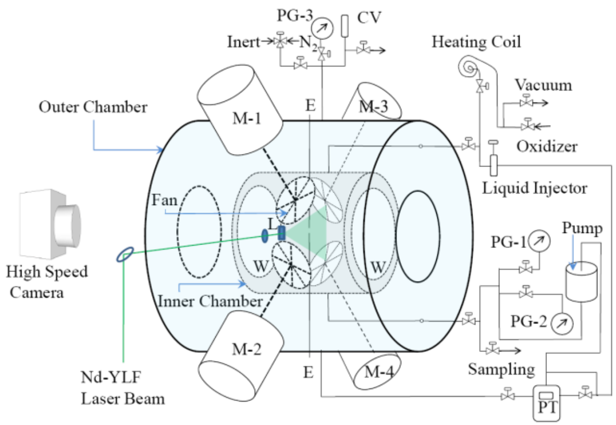
t = 0 µs t = 111 µs t = 222 µs t = 333 µs t = 444 µs

Major data set obtained over range of velocities (4-70 m/s), pressures (1-20 atm), turbulence intensities, fuel compositions. S_T/S_L can be >>100.

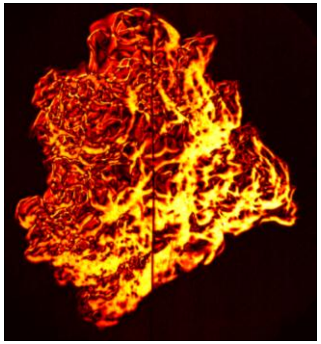
No upper limits observed in turbulence flame speed!!!
Much more efficient and compacted combustor can be designed.

More Turbulent Flame Experiments

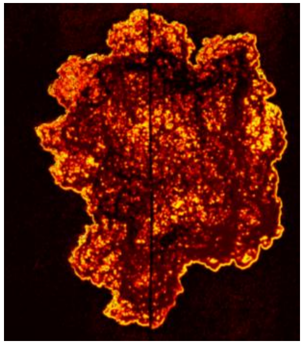
Flame Speed and Self-similar Propagation of Turbulent Premixed Flames: (PI: Law, Princeton)



CV: Check Valve, PG: Pressure Gauge, PT: Pressure Transducer, M: Fan Motor, L: Cylindrical Lens, E: Electrodes, W: Quartz Window

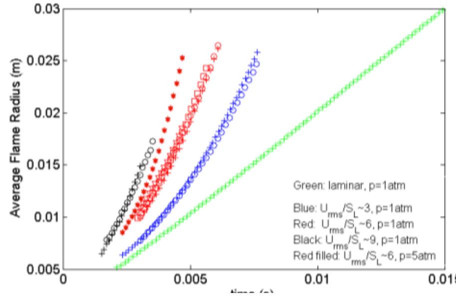


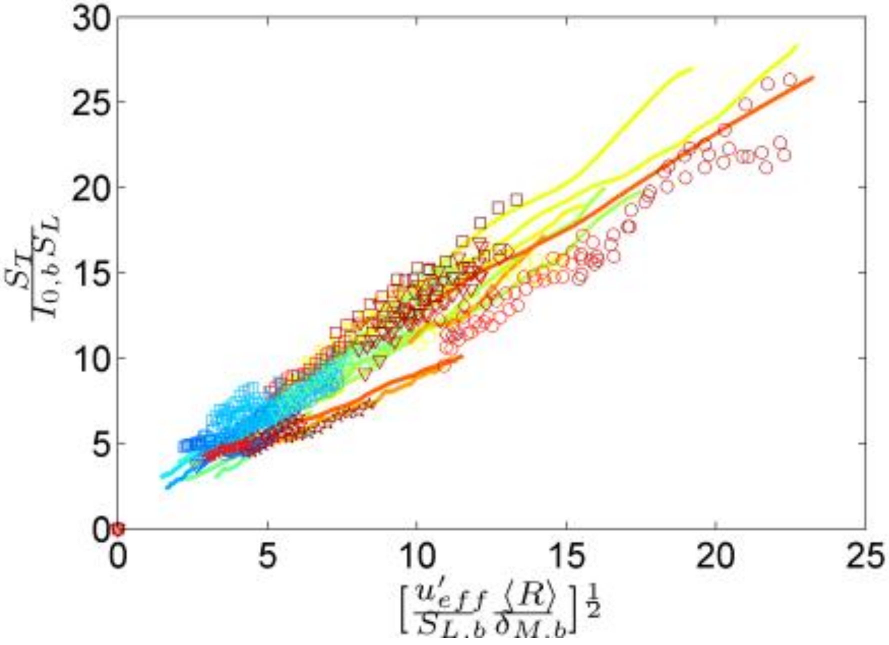
Pressure = 1atm



Pressure = 5atm

Schlieren images of turbulent premixed CH_4-air flames (ϕ=0.9, Le=1) at same u_{rms}



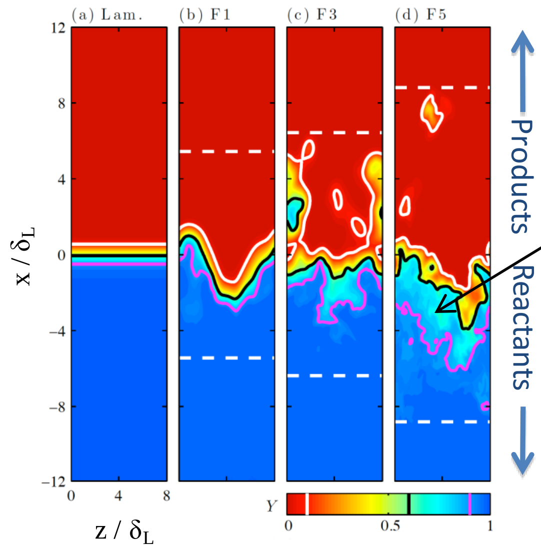


Turbulence flame speed can be scaled, at least partially understood and modeled.

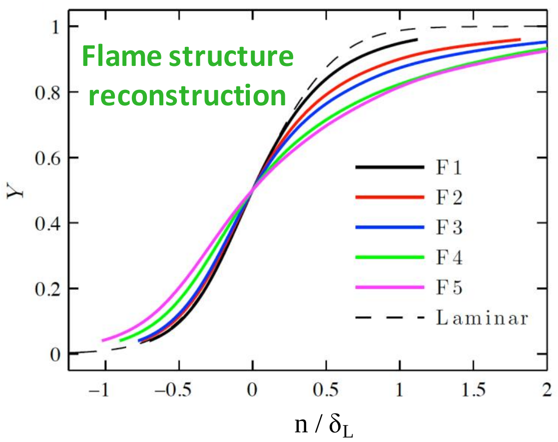
Turbulent Flame Interactions

Turbulent Flame Structure: (PIs: Oran, Poludnenko & Hamlington NRL)

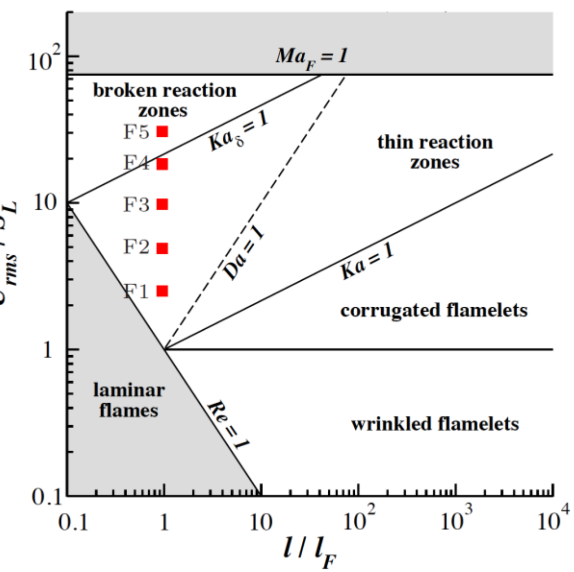
Domain cross-sections



thicken pre-heating (pyrolysis) zone



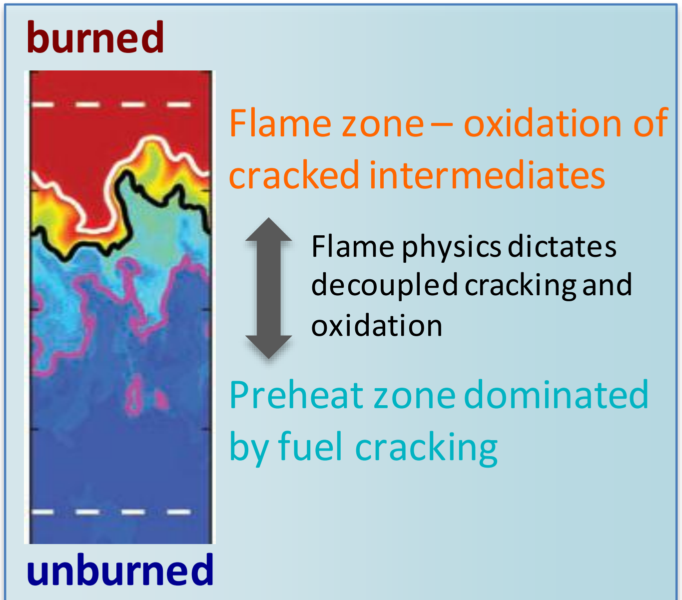
Combustion regime diagram showing performed simulations

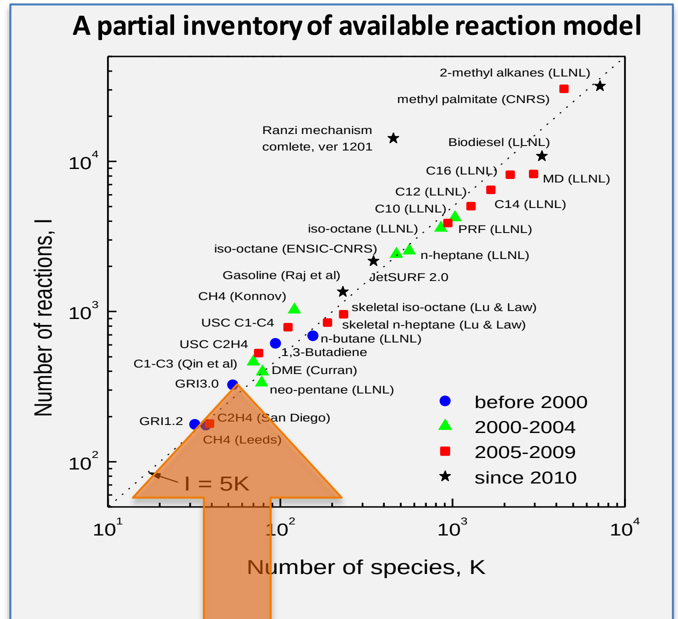


- **small turbulent intensity, f**
- **large intensities, preheat (pyrolysis) zone broadened and reaction zone virtually unaffected**
- **robustness of reaction zone – turbulent diffusion suppressed in reaction zone by heat release (suppressed small scales)**
- **tangential strain rate thins flame**

We may be able to understand turbulent flame structure after all…

Turbulence-Chemistry Interaction





Stage 1: quantify the pyrolysis process in the thicken pre-heating zone, which leads to ~6 c1-c4 molecular fragments

Stage 2: combined with the c1-c4 combustion chemistry that has been well characterized.

Turbulence-Chemistry Interaction: (PI: Wang, USC)

Turbulent Pre-Heating (Pyrolysis) Zone Makes the Chemistry Model Simpler….

Turbulent Flame Property: Where We Are

With recent developments in combustion diagnostics and numerical simulation for the reactive flow, we begun to observe and understand fundamental attributes of the turbulent flame in Air-Force-relevant realms,

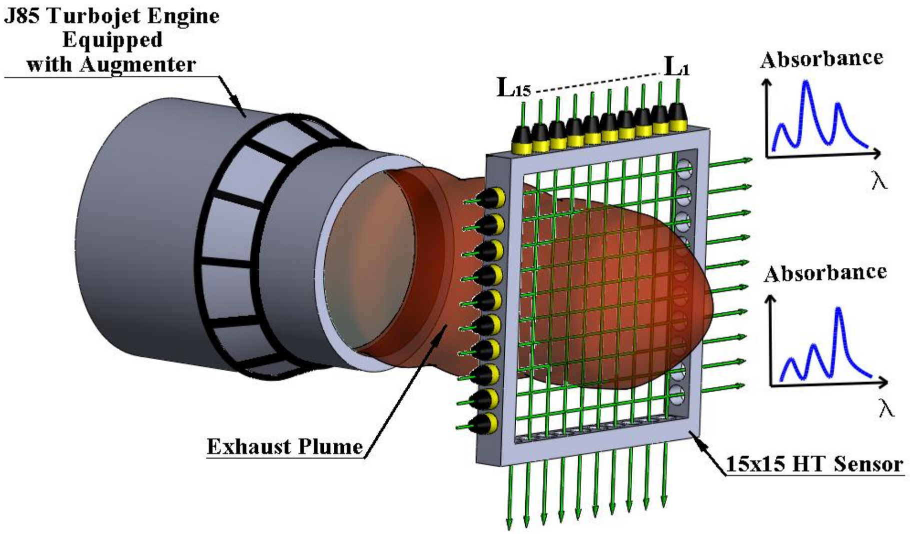
Leading to:

- Quantify of interactions among different scales
- Establish of usable turbulent combustion models
- With acceptable uncertainty to revolutionized Air Force propulsion system development.

Examples of Continuous Transition

Diagnostics

State-of-Art Optical Fibers, Probes, Single-Beam Techniques



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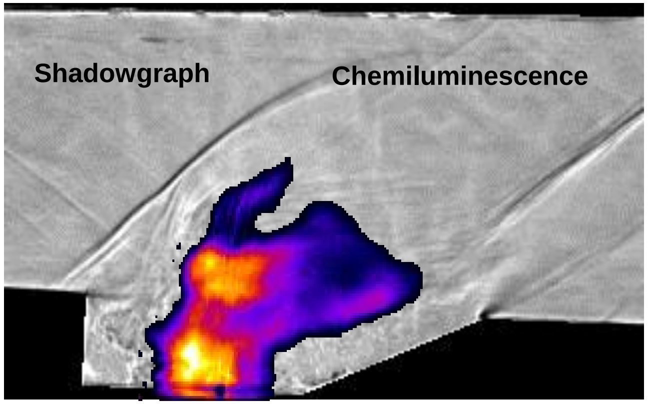
Basic Combustion

New Ignition Technique



Closing Statements

After a year, the portfolio is taking shape.

Supported projects have started showing very encouraging results.

More to come, stay tuned.